

368866

*Priority*  
*8/10/98*

Trying 3106016892...Open

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LOGINID:ssspta1200jxo  
PASSWORD:  
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NEWS	1	Feb	2	Web Page URLs for STN Seminar Schedule - N. America
NEWS	2	Dec	17	Expanded CAPLUS Coverage of US, Japanese, WIPO, EPO, and German patents
NEWS	3	Feb	1	Addition of Machine-Translated Abstracts to CAPLUS
NEWS	4	Feb	28	Patent Information Now Searchable in CAOLD SDI/UPDATE SEARCH FIELD
NEWS	5	May	1	Beilstein Abstracts on STN - FILE BABS
NEWS	6	May	1	RN CROSSOVER AND ANSWER SIZE LIMITS INCREASED
NEWS	7	May	1	AIDSLINE has been reloaded
NEWS	8	May	1	Searching Y2-K compliant Patent Numbers
NEWS	9	May	9	Sequence Similarity Batch Search in DGENE
NEWS	10	May	19	Weekly Statistics for New Entries now available in INPADOC
NEWS	11	May	22	CITED REFERENCES NOW AVAILABLE IN CAPLUS AND CA FILE
NEWS	12	May	22	POSTPROCESSING OF SEARCH RESULTS MAY BE AFFECTED BY ADDITION OF CITED REFERENCES TO CAPLUS, CA, REGISTRY, CASREACT, MARPAT, and MARPATPREV
NEWS	13	Jun	2	KOREAN PATENTS NOW IN CAS DATABASES
NEWS	14	Jun	20	WIPO/PCT Patents Fulltext Database now on STN
NEWS	15	Jun	28	NEWS 15 Jun 28 CAS covers Web-distributed preprints
NEWS	16	Jul	7	Patent Full-text Cluster, PNTTEXT, introduced
NEWS EXPRESS	FREE UPGRADE 5.0C NOW AVAILABLE			
NEWS HOURS	STN Operating Hours Plus Help Desk Availability			
NEWS INTER	General Internet Information			
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NEWS PHONE	Direct Dial and Telecommunication Network Access to STN			
NEWS WWW	CAS World Wide Web Site (general information)			

Enter NEWS followed by the item number or name to see news on that specific topic.

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\* \* \* \* \* STN Columbus \* \* \* \* \*

FILE 'HOME' ENTERED AT 12:15:13 ON 20 JUL 2000

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.15	0.15

FILE 'REGISTRY' ENTERED AT 12:15:18 ON 20 JUL 2000

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STRUCTURE FILE UPDATES: 19 JUL 2000 HIGHEST RN 278777-27-8

DICTIONARY FILE UPDATES: 19 JUL 2000 HIGHEST RN 278777-27-8

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 11, 2000

Please note that search-term pricing does apply when  
conducting SmartSELECT searches.

Structure search limits have been increased. See HELP SLIMIT  
for details.

\*\*\* YOU HAVE NEW MAIL \*\*\*

=>

Uploading 368866.str

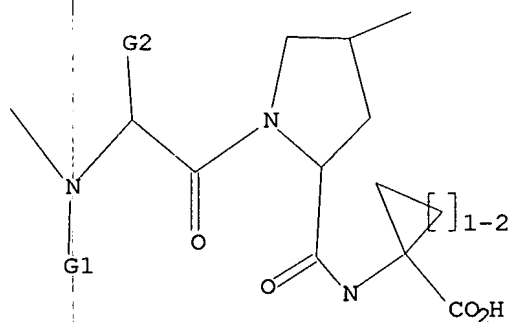
L1 STRUCTURE UPLOADED

=> d L1

L1 HAS NO ANSWERS

L1 STR

368866



G1 C, H, Me, Et, n-Pr, i-Pr, n-Bu, i-Bu, t-Bu

G2 C, H, Cb, Ak

Structure attributes must be viewed using STN Express query preparation.

=> s L1 sss full

FULL SEARCH INITIATED 12:15:58 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 35 TO ITERATE

100.0% PROCESSED 35 ITERATIONS  
SEARCH TIME: 00.00.01

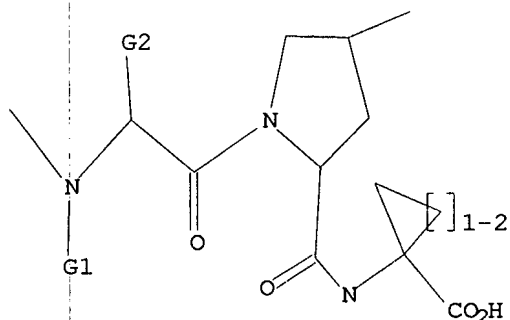
0 ANSWERS

L2 0 SEA SSS FUL L1

=> d L1

L1 HAS NO ANSWERS  
L1 STR

368866



G1 C,H,Me,Et,n-Pr,i-Pr,n-Bu,i-Bu,t-Bu

G2 C,H,Cb,Ak

Structure attributes must be viewed using STN Express query preparation.

=> file beil

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	126.60	126.75

FILE 'BEILSTEIN' ENTERED AT 12:16:19 ON 20 JUL 2000  
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Beilstein Informationssysteme GmbH

FILE LAST UPDATED: 6 MAR 2000

FILE COVERS 1779 TO 2000.

\*\*\* CAS REGISTRY NUMBERS FOR 4,356,237 SUBSTANCES AVAILABLE \*\*\*

\*\*\* FILE CONTAINS 7,688,486 SUBSTANCES \*\*\*

\*\*\*\*\*  
\* PLEASE NOTE THAT THERE ARE NO FORMATS FREE OF COST. \*  
\* SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE \*  
\* ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE; THESE \*  
\* ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS. \*  
\* FOR PRICE INFORMATION SEE HELP COST \*  
\*\*\*\*\*

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\*\*\* YOU HAVE NEW MAIL \*\*\*

=> s L1 full

FULL SEARCH INITIATED 12:16:32 FILE 'BEILSTEIN'  
FULL SCREEN SEARCH COMPLETED - 0 TO ITERATE

100.0% PROCESSED 0 ITERATIONS 0 ANSWERS  
SEARCH TIME: 00.00.03

L3 0 SEA SSS FUL L1

=> file caslink

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.00	126.75

FILE 'REGISTRY' ENTERED AT 12:16:41 ON 20 JUL 2000  
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FILE 'MARPAT' ENTERED AT 12:16:41 ON 20 JUL 2000  
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\*\*\* YOU HAVE NEW MAIL \*\*\*

CLUSTER 'CASLINK' ENTERED

Predefined command sequences will be executed in  
REGISTRY, MARPAT, MARPATPREV, and CAPLUS.

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=> s L1 full

S L1 SSS FUL FILE=REGISTRY  
FULL SEARCH INITIATED 12:17:42 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 35 TO ITERATE

100.0% PROCESSED 35 ITERATIONS 0 ANSWERS  
SEARCH TIME: 00.00.01

L4 0 SEA SSS FUL L1  
1 FILES SEARCHED...

S L4 SSS FUL FILE=MARPAT  
FULL SEARCH INITIATED 12:17:45 FILE 'MARPAT'  
FULL SCREEN SEARCH COMPLETED - 20573 TO ITERATE

8.1% PROCESSED	1668 ITERATIONS		0 ANSWERS
15.9% PROCESSED	3268 ITERATIONS	( 1 INCOMPLETE)	1 ANSWERS
21.8% PROCESSED	4475 ITERATIONS	( 1 INCOMPLETE)	1 ANSWERS
25.2% PROCESSED	5184 ITERATIONS	( 1 INCOMPLETE)	1 ANSWERS
31.5% PROCESSED	6476 ITERATIONS	( 1 INCOMPLETE)	2 ANSWERS
42.7% PROCESSED	8779 ITERATIONS	( 2 INCOMPLETE)	4 ANSWERS
53.8% PROCESSED	11070 ITERATIONS	( 2 INCOMPLETE)	4 ANSWERS
61.0% PROCESSED	12557 ITERATIONS	( 2 INCOMPLETE)	4 ANSWERS
68.3% PROCESSED	14045 ITERATIONS	( 3 INCOMPLETE)	5 ANSWERS
74.5% PROCESSED	15323 ITERATIONS	( 4 INCOMPLETE)	6 ANSWERS
80.1% PROCESSED	16485 ITERATIONS	( 4 INCOMPLETE)	6 ANSWERS
85.6% PROCESSED	17609 ITERATIONS	( 5 INCOMPLETE)	8 ANSWERS
90.1% PROCESSED	18544 ITERATIONS	( 5 INCOMPLETE)	8 ANSWERS
93.1% PROCESSED	19147 ITERATIONS	( 5 INCOMPLETE)	8 ANSWERS
94.9% PROCESSED	19529 ITERATIONS	( 5 INCOMPLETE)	8 ANSWERS

368866

95.8% PROCESSED	19712 ITERATIONS	( 5 INCOMPLETE)	8 ANSWERS
96.3% PROCESSED	19817 ITERATIONS	( 5 INCOMPLETE)	8 ANSWERS
96.7% PROCESSED	19885 ITERATIONS	( 5 INCOMPLETE)	8 ANSWERS
97.2% PROCESSED	19992 ITERATIONS	( 5 INCOMPLETE)	8 ANSWERS
97.5% PROCESSED	20066 ITERATIONS	( 5 INCOMPLETE)	8 ANSWERS
97.8% PROCESSED	20129 ITERATIONS	( 5 INCOMPLETE)	8 ANSWERS
98.8% PROCESSED	20335 ITERATIONS	( 5 INCOMPLETE)	8 ANSWERS
99.4% PROCESSED	20441 ITERATIONS	( 5 INCOMPLETE)	8 ANSWERS
100.0% PROCESSED	20573 ITERATIONS	( 5 INCOMPLETE)	8 ANSWERS

SEARCH TIME: 00.06.41

L5                8 SEA SSS FUL L1  
1 FILES SEARCHED...

S L5 SSS FUL FILE=MARPATPREV  
FULL SEARCH INITIATED 12:24:28 FILE 'MARPATPREV'  
FULL SCREEN SEARCH COMPLETED - 100 TO ITERATE

100.0% PROCESSED	100 ITERATIONS	0 ANSWERS
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SEARCH TIME: 00.00.07

L6                0 SEA SSS FUL L1  
1 FILES SEARCHED...

S L4 FILE=CAPLUS  
L7                0 FILE CAPLUS  
1 FILES SEARCHED...

SET DUPORDER FILE  
SET COMMAND COMPLETED

DUP REM L6 L5 L7  
L6 HAS NO ANSWERS  
L7 HAS NO ANSWERS  
PROCESSING COMPLETED FOR L6  
PROCESSING COMPLETED FOR L5  
PROCESSING COMPLETED FOR L7  
L8                8 DUP REM L6 L5 L7 (0 DUPLICATES REMOVED)  
                  ANSWERS '1-8' FROM FILE MARPAT

368866

=> d L8 1-8 ibib abs FHIT

L8 ANSWER 1 OF 8 MARPAT COPYRIGHT 2000 ACS

ACCESSION NUMBER: 132:175808 MARPAT

TITLE: Hepatitis C inhibitor peptides

INVENTOR(S): Llinas-Brunet, Montse; Bailey, Murray D.; Cameron, Dale; Ghio, Elise; Goudreau, Nathalie; Poupart, Marc-Andre; Rancourt, Jean; Tsantrizos, Youla S.

PATENT ASSIGNEE(S): Boehringer Ingelheim (Canada) Ltd., Can.

SOURCE: PCT Int. Appl., 113 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

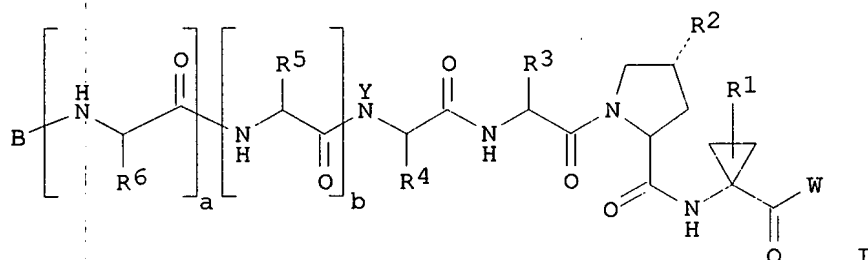
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000009558	A1	20000224	WO 1999-CA737	19990809
<p>W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM</p> <p>RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG</p>				
AU 9952732	A1	20000306	AU 1999-52732	19990809
PRIORITY APPLN. INFO.:			US 1998-95945	19980810
			WO 1999-CA737	19990809

GI

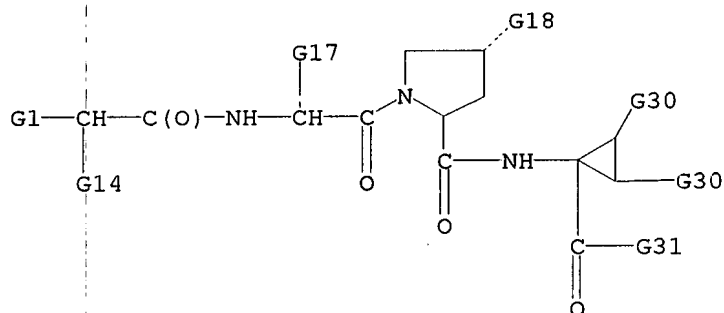




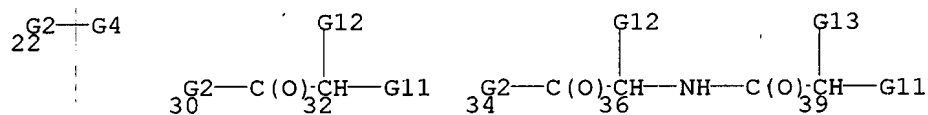
368866

AB The invention provides peptides I (a, b = 0, 1; Y = H, C1-6 alkyl; B = H, acyl deriv., sulfonyl deriv.; W = OH, N-substituted amino), or a pharmaceutically acceptable salt or ester thereof, for use in the treatment of hepatitis C virus infection. Prepn. of peptides is included.

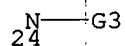
**MSTR 1**



G1 = NH<sub>2</sub> / 22 / 30 / 34

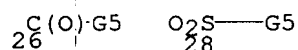


G2 = NH / 24



G3 = alkyl<(1-6)> / (SC Me)

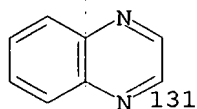
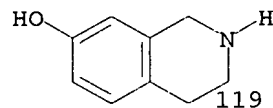
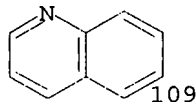
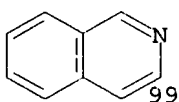
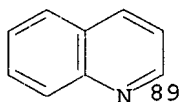
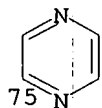
G4 = 26 / 28 / (SC COMe)



G5 = alkyl<(1-10)> (SO G6) / cycloalkyl<(3-7)> (SO G7) / aryl<(6-10)> (SO G8) / alkyl<(1-6)> (SR (1-) G9) /

368866

Hy<EC (5-) A (1-4) Q (0-) O (0-) S (0-) N (0) OTHERQ,  
RC (1-), RS (0-) E5 (0-) E6 (0-) E7> (SO G10) / (SC 75 / 89 /  
99 / 109 / 119 / 131)



G6 = CO2H / alkylcarbonyloxy<(1-5)> / OCHO /  
alkoxy<(1-6)>  
G7 = CO2H / alkoxycarbonyl<(1-6)> / CO2CH2Ph  
G8 = alkyl<(1-6)> / OH / NH2 / alkylamino<(1-6)> /  
dialkylamino<(1-6)>  
G9 = aryl<(6-10)> (SO G8)  
G10 = alkyl<(1-6)> / OH / NH2 / alkylamino<(1-6)> /  
dialkylamino<(1-6)> / CONH2 / alkylaminocarbonyl<(1-6)> /  
dialkylaminocarbonyl<(1-6)>  
G11 = NH2 / 41

HN—G4  
41

G12 = alkyl<(1-6)> (SO CO2H) / (SC CH2CO2H / CH2CH2CO2H /  
Pr-i / Bu-t)  
G13 = alkyl<(1-6)> (SR CO2H) / (SC CH2CO2H / CH2CH2CO2H)  
G14 = alkyl<(1-10)> / cycloalkyl<(3-7)> / 47 / (SC Pr-i /  
cyclohexyl / Bu-t / Bu-s / Bu-i)

G15—G16  
47

G15 = alkylene<(1-7)>  
G16 = cycloalkyl<(3-7)>  
G17 = **alkyl<(1-10)>** / cycloalkyl<(3-7)> / 50 / (SC Bu-s /  
cyclohexyl / Pr-i / Bu-t)

368866

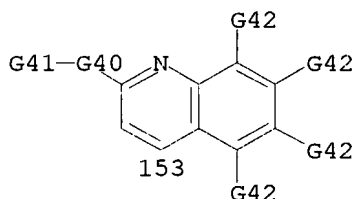
G15-G16  
50

G18 = 53 / 57

H<sub>2</sub>C-G39 G23-G19  
53 57

G19 = Cb<(3-7)> (SO (1-3) G20) / 55 /  
aryl<(6-10)> (SO (1-3) G20) / alkyl<(1-6)> (SR (1-) G24) /  
Hy<EC (5-) A (1-4) Q (0-) O (0-) S (0-) N (0) OTHERQ,  
RC (1-), RS (0-) E5 (0-) E6 (0-) E7> (SO (1-3) G20) / 59 /  
(SC 133 / naphthyl / quinolinyll (SO (1-2) G34) / 153)

G21-G22 G32-G25 H<sub>2</sub>C-G33  
55 59 133



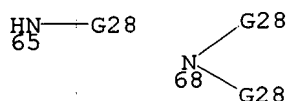
G20 = alkyl<(1-6)> / alkoxy<(1-6)> / NH2 /  
alkylamino<(1-6)> / dialkylamino<(1-6)> / 61 / NO2 / OH /  
SH / F / Cl / Br / I / alkyl (SR (1-) G26) / 63 / CO2H /  
alkyl<(1-6)> (SR CO2H) / aryl<(6-10)> (SO) /  
alkyl<(1-6)> (SR (1-) aryl<(6-10)> (SO)) /  
Hy<EC (5-) A (1-4) Q (0-) O (0-) S (0-) N (0) OTHERQ,  
RC (1-), RS (0-) E5 (0-) E6 (0-) E7> (SO)

O<sub>2</sub>S-R C(O)-G27  
61 63

G21 = Ak<(1-7)>  
G22 = Cb<(3-7)> (SO (1-3) G20)  
G23 = NH / O / S  
G24 = aryl<(6-10)> (SO (1-3) G20)  
G25 = Hy<EC (5-) A (1-4) Q (0-) O (0-) S (0-) N (0)  
OTHERQ, RC (1-), RS (0-) E5 (0-) E6 (0-) E7> (SO (1-3) G20)  
G26 = F / Cl / Br / I

368866

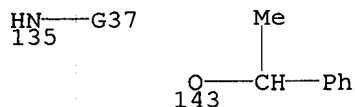
G27 = NH2 / 65 / 68



G28 = alkyl<(1-6)> / aryl<(6-10)> (SO) /  
 alkyl<(1-6)> (SR (1-) aryl<(6-10)> (SO)) /  
 Hy<EC (5-) A (1-4) Q (0-) O (0-) S (0-) N (0) OTHERQ,  
 RC (1-), RS (0-) E5 (0-) E6 (0-) E7> (SO) / 70

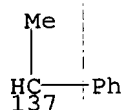
~~G32-G29~~  
70

G29 = Hy<EC (5-) A (1-4) Q (0-) O (0-) S (0-) N (0)  
 OTHERQ, RC (1-), RS (0-) E5 (0-) E6 (0-) E7> (SO)  
 G30 = (1-) H / alkyl<(1-6)> (SO (1-) G26) /  
 alkenyl<(2-6)> (SO (1-) G26) / (SC Me (SO (1-) G26) /  
 Et (SO (1-) G26) / Pr-n (SO (1-) G26) / CH=CH2 (SO (1-) G26))  
 G31 = OH (SO) / NH2 (SR) / (SC 135 /  
 alkoxy<(1-6)> (SO (1-) aryl<(6-10)>) / OPh / OMe / OEt /  
 OCH2Ph / 143)



G32 = alkylene<(1-6)>  
 G33 = naphthyl / Ph  
 G34 = CONH2 / alkylaminocarbonyl<(1-6)> /  
 dialkylaminocarbonyl<(1-6)> / aryl<(6-10)> (SO G35) /  
 alkyl<(1-6)> (SR (1-) G36) / Hy<EC (5-) A (1-4) Q (0-) O (0-)  
 S (0-) N (0) OTHERQ, RC (1-), RS (0-) E5 (0-) E6 (0-) E7>  
 (SO G35) / alkyl<(1-6)> / alkoxy<(1-6)> / NH2 /  
 dialkylamino<(1-6)> / alkylcarbonylamino<(1-6)> / NO2 / OH /  
 F / Cl / Br / I / CF3 / CO2H / OMe / NHCOMe  
 G35 = NH2 / dialkylamino<(1-6)> /  
 alkylcarbonylamino<(1-6)> / NMe2 / NHCOMe  
 G36 = aryl<(6-10)> (SO G35)  
 G37 = CH2Ph / 137

368866



G39 = Cb<(3-7)> (SO (1-3) G20) / 144 /  
aryl<(6-10)> (SO (1-3) G20) / alkyl<(1-6)> (SR (1-) G24) /  
Hy<EC (5-) A (1-4) Q (0-) O (0-) S (0-) N (0) OTHERQ,  
RC (1-), RS (0-) E5 (0-) E6 (0-) E7> (SO (1-3) G20) / 146

G21-G22 G32-G25  
144 146

G40 = phenylene / Hy<EC (5-) A (1-4) Q (0-) O (0-) S (0-)  
N (0) OTHERQ, RC (1-), RS (0-) E5 (0-) E6 (0-) E7>  
G41 = NH2 / dialkylamino<(1-6)> /  
alkylcarbonylamino<(1-6)> / NO2 / OH / F / Cl / Br / I /  
CF3 / CO2H  
G42 = (3-) H / NHCOMe / F / Cl / Br / I / NH2 / NO2 /  
alkoxy<(1-6)> / OMe  
DER: or pharmaceutically acceptable salts or esters  
MPL: claim 1  
STE: 32,36,39 - D,L  
STE: and racemates, diastereoisomers and optical isomers

REFERENCE COUNT: 5

REFERENCE(S):

- (1) Boehringer Ingelheim Canada Ltd; WO 9907733 A2  
1999 CAPLUS
- (2) Ingallinella, P; Biochemistry 1998, V37, P8906  
CAPLUS
- (3) Linas-Brunet, M; Bioorganic & Medicinal Chemistry  
Letters 1998, V8, P1713
- (4) Mori, A; Biochemical and biophysical research  
communications 1997, V231, P738 CAPLUS
- (5) Vertex Pharmaceuticals Incorporated; WO 9817679

A1

1998 CAPLUS

L8 ANSWER 2 OF 8 MARPAT COPYRIGHT 2000 ACS

ACCESSION NUMBER: 132:180871 MARPAT

TITLE: Preparation of hepatitis C inhibitory tripeptides

INVENTOR(S): Llinas-Brunet, Montse; Bailey, Murray D.; Cameron,  
Dale; Faucher, Anne-Marie; Ghio, Elise; Goudreau,

*Applicants*

368866

Nathalie; Halmos, Teddy; Poupart, Marc-Andre;  
 Rancourt, Jean; Tsantrizos, Youla S.; Wernic, Dominik  
 M.; Simoneau, Bruno  
 PATENT ASSIGNEE(S): Boehringer Ingelheim (Canada) Ltd., Can.  
 SOURCE: PCT Int. Appl., 168 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000009543	A2	20000224	WO 1999-CA736	19990809
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 9952731	A1	20000306	AU 1999-52731	19990809
PRIORITY APPLN. INFO.:			US 1998-95931	19980810
			US 1999-132386	19990504
			WO 1999-CA736	19990809

GI

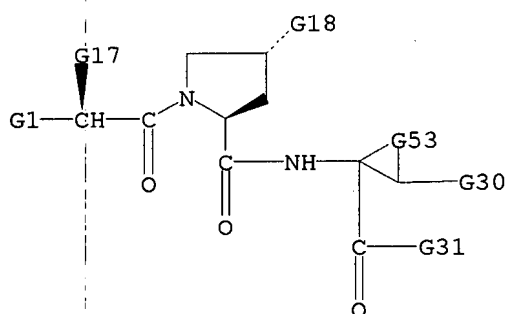
\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Peptides I [B = H, (un)substituted aryl, aralkyl, heterocyclyl, or  
 alkylheterocyclyl, acyl R4CO, carboxylate R4O2C, amide R4NR5CO, thioamide  
 R4NR5C(S), or sulfonyl group R4SO2, where R4 = (un)substituted alkyl,  
 cycloalkyl, cycloalkoxy, amino, aralkyl, or heterocyclyl, with proviso  
 that R4 .noteq. cycloalkoxy for amides or thioamides; R5, Y = H, alkyl;  
 R3 = (un)substituted alkyl, cycloalkyl, or alkylcycloalkyl; R2 =  
 (un)substituted cycloalkyl-, aryl-, aralkyl-, or heterocyclylmethyl,  
 -amino, -oxy, or -thio; R1 = H; alkyl, cycloalkyl, alkenyl, or alkynyl,  
 all optionally substituted with halogen] or their racemates,  
 diastereoisomers, and optical isomers were prepd. as hepatitis C virus  
 (HCV) inhibitory tripeptides. Thus, compd. II was prepd. via peptide  
 coupling reactions in soln. and showed IC50 < 0.5 .mu.M in the  
 recombinant

368866

HCV NS3 protease/NS4A cofactor peptide radiometric assay.

MSTR 1



G1 = NH2 / 22 / alkylamino<(1-6)> / (SC NHMe)

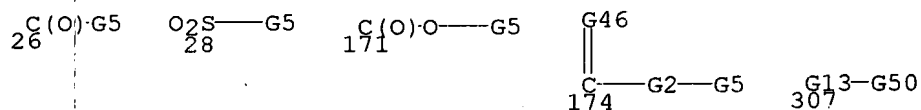
G2—G4  
22

G2 = NH / 24

N—G3  
24

G3 = alkyl<(1-6)> / (SC Me)

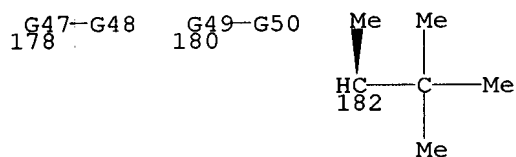
G4 = aryl<(6-10)> (SO G11) / alkyl<(1-6)> (SR (1-) G12) /  
Hy<EC (5-) A (1-4) Q (0-) O (0-) S (0-) N (0) OTHERQ,  
RC (1-), RS (0-) E5 (0-) E6 (0-) E7> (SO G11) / 307 / 26 /  
28 / 171 / 174 / (SC COMe)



G5 = alkyl<(1-10)> (SO G6) / cycloalkyl<(3-7)> (SO G7) /  
cycloalkyloxy<(3-7)> (SO G7) / 178 / NH2 /  
alkylamino<(1-6)> / dialkylamino<(1-6)> / CONH2 /  
alkylcarbonylamino<(1-6)> / aryl<(6-10)> (SO G8) /  
alkyl<(1-6)> (SR (1-) G9) / Hy<EC (5-) A (1-4) Q (0-) O (0-)

368866

S (0-) N (0) OTHERQ, RC (1-), RS (0-) E5 (0-) E6 (0-) E7>  
(SO G10) / 180 / (SC Bu-t / 182)



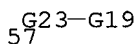
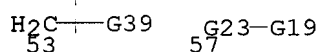
G6 = CO2H / alkylcarbonyl<(1-5)> / CHO / OH /  
alkoxy<(1-6)> / NH2 / alkylamino<(1-6)> /  
dialkylamino<(1-6)> / CONH2 / alkylaminocarbonyl<(1-6)>  
G7 = OH / CO2H / alkoxy<(1-6)> / NH2 /  
alkylamino<(1-6)> / dialkylamino<(1-6)> / CONH2 /  
alkylaminocarbonyl<(1-6)>  
G8 = alkyl<(1-6)> / OH / CONH2 /  
alkylaminocarbonyl<(1-6)> / NH2 / alkylamino<(1-6)> /  
dialkylamino<(1-6)>  
G9 = aryl<(6-10)> (SO G8)  
G10 = alkyl<(1-6)> / OH / CONH2 /  
alkylaminocarbonyl<(1-6)> / NH2 / alkylamino<(1-6)> /  
dialkylamino<(1-6)>  
G11 = alkyl<(1-6)> (SO (1-) G26) / alkoxy<(1-6)> /  
alkylcarbonyl<(1-5)> / CHO / OH / alkyl<(1-6)> (SR OH) /  
NO2 / CN / alkyl<(1-6)> (SR CN) / NH2 / alkylamino<(1-6)> /  
dialkylamino<(1-6)> / CONH2 / alkylaminocarbonyl<(1-6)>  
G12 = aryl<(6-10)> (SO G11)  
G13 = Hy<EC (5-) A (1-4) Q (0-) O (0-) S (0-) N (0)  
OTHERQ, RC (1-), RS (0-) E5 (0-) E6 (0-) E7> (SO G11)  
G14 = OH / alkoxy<(1-6)> / alkylthio<(1-6)> / CONH2 /  
alkylaminocarbonyl<(1-6)> / aryl<(6-10)> /  
alkyl<(1-6)> (SR (1-) aryl<(6-10)>)  
G15 = alkylene<(1-7)> (SO (1-) G14)  
G16 = cycloalkyl<(3-7)> (SO (1-) G14)  
G17 = **alkyl<(1-8)> (SO (1-) G14)** /  
cycloalkyl<(3-7)> (SO (1-) G14) / 50 / (SC Bu-s /  
cyclohexyl / Pr-i / Bu-t)

G15-G16  
50

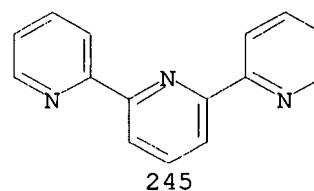
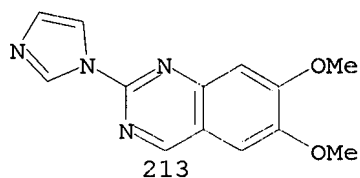
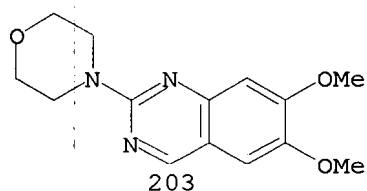
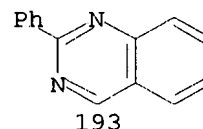
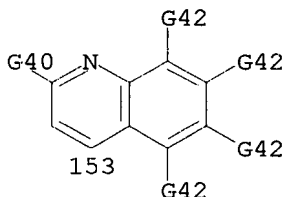
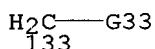
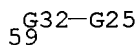
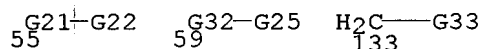
G18 = 53 / 57



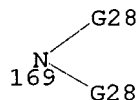
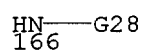
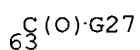
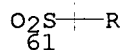
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G19 = Cb<(3-7)> (SO (1-3) G20) / 55 /  
 aryl<(6-10)> (SO (1-3) G20) / alkyl<(1-6)> (SR (1-) G24) /  
 Hy<EC (5-) A (1-4) Q (0-) O (0-) S (0-) N (0) OTHERQ,  
 RC (1-), RS (0-) E5 (0-) E6 (0-) E7> (SO (1-3) G20) / 59 /  
 (SC 133 / naphthyl / quinoliny1 (SO (1-) G34) / 193 / 203 /  
 213 / 245 / 153)

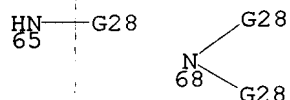


G20 = alkyl<(1-6)> / alkoxy<(1-6)> / alkylthio<(1-6)> /  
 NH2 / 61 / 166 / 169 / NO2 / OH / SH / F / Cl / Br / I /  
 alkyl (SR (1-) G26) / 63 / CO2H / alkyl<(1-6)> (SR CO2H) /  
 aryl<(6-10)> (SO) / alkyl<(1-6)> (SR (1-) aryl<(6-10)>  
 (SO)) / Hy<EC (5-) A (1-4) Q (0-) O (0-) S (0-) N (0)  
 OTHERQ, RC (1-), RS (0-) E5 (0-) E6 (0-) E7> (SO)



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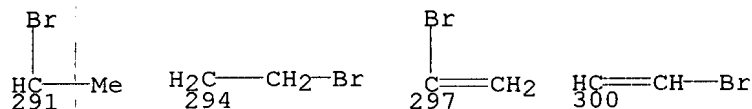
G21 = Ak<(1-7)>  
 G22 = Cb<(3-7)> (SO (1-3) G20)  
 G23 = NH / O / S  
 G24 = aryl<(6-10)> (SO (1-3) G20)  
 G25 = Hy<EC (5-) A (1-4) Q (0-) O (0-) S (0-) N (0)  
 OTHERQ, RC (1-), RS (0-) E5 (0-) E6 (0-) E7> (SO (1-3) G20)  
 G26 = F / Cl / Br / I  
 G27 = NH2 / 65 / 68



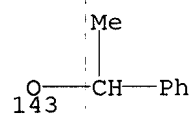
G28 = alkyl<(1-6)> / aryl<(6-10)> (SO) /  
 alkyl<(1-6)> (SR (1-) aryl<(6-10)> (SO)) /  
 Hy<EC (5-) A (1-4) Q (0-) O (0-) S (0-) N (0) OTHERQ,  
 RC (1-), RS (0-) E5 (0-) E6 (0-) E7> (SO) / 70

~~G32-G29~~  
 70

G29 = Hy<EC (5-) A (1-4) Q (0-) O (0-) S (0-) N (0)  
 OTHERQ, RC (1-), RS (0-) E5 (0-) E6 (0-) E7> (SO)  
 G30 = (1-) H / alkyl<(1-6)> (SO (1-) G26) /  
 alkenyl<(2-6)> (SO (1-) G26) / cycloalkyl<(3-7)>  
 (SO (1-) G26) / alkynyl<(2-6)> (SO (1-) G26) / (SC Et /  
 CH=CH2 / cyclopropyl / 291 / 294 / 297 / 300)



G31 = OH (SO) / (SC alkoxy<(1-6)> (SO (1-) aryl<(6-10)>)) /  
 OPh / OMe / OEt / OCH2Ph / 143)



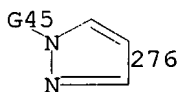
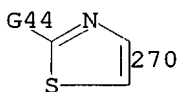
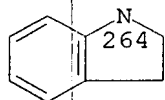
G32 = alkylene<(1-6)> / (SC CH2)

368866

G33 = naphthyl / Ph  
 G34 = R / Cl / OMe / CF3 / NH2  
 G39 = Cb<(3-7)> (SO (1-3) G20) / 144 /  
 aryl<(6-10)> (SO (1-3) G20) / alkyl<(1-6)> (SR (1-) G24) /  
 Hy<EC (5-) A (1-4) Q (0-) O (0-) S (0-) N (0) OTHERQ,  
 RC (1-), RS (0-) E5 (0-) E6 (0-) E7> (SO (1-3) G20) / 146

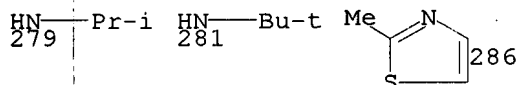
G21-G22 G32-G25  
 144 146

G40 = alkyl<(1-6)> / alkoxy<(1-6)> / alkylthio<(1-6)> /  
 F / Cl / Br / I / NH2 / alkylamino<(1-6)> /  
 dialkylamino<(1-6)> / aryl<(6-10)> (SO G41) /  
 alkyl<(1-6)> (SR (1-) G43) / Hy<EC (5-) A (1-4) Q (0-) O (0-)  
 S (0-) N (0) OTHERQ, RC (1-), RS (0-) E5 (0-) E6 (0-) E7>  
 (SO G41) / 264 / 270 / 276 / 289



G51-G52  
 289

G41 = alkyl<(1-6)> / alkoxy<(1-6)> / CONH2 /  
 alkylaminocarbonyl<(1-6)> / NH2 / alkylamino<(1-6)> /  
 dialkylamino<(1-6)> / Hy<EC (5-) A (1-4) Q (0-) O (0-) S (0-)  
 N (0) OTHERQ, RC (1-), RS (0-) E5 (0-) E6 (0-) E7>  
 G42 = (3-) H / alkyl<(1-6)> / alkoxy<(1-6)> / NH2 /  
 dialkylamino<(1-6)> / alkylaminocarbonyl<(1-6)> / NO2 / OH /  
 F / Cl / Br / I / CF3 / CO2H / OMe  
 G43 = aryl<(6-10)> (SO G41)  
 G44 = Me / Et / NHMe / NHCOMe / NH2 / NHET / 279 / 281 /  
 286 / alkyl<(1-6)> / alkylamino<(1-6)> /  
 dialkylamino<(1-6)> / CONH2 / alkylaminocarbonyl<(1-6)>



G45 = Me / Bu-t  
 G46 = O / S  
 G47 = alkylene<(1-7)>  
 G48 = cycloalkyl<(3-7)> (SO G7)  
 G49 = alkylene<(1-6)>

368866


G50 = Hy<EC (5-) A (1-4) Q (0-) O (0-) S (0-) N (0)  
OTHERQ, RC (1-), RS (0-) E5 (0-) E6 (0-) E7> (SO G10)  
G51 = phenylene  
G52 = alkyl<(1-6)> / alkoxy<(1-6)> / F / Cl / Br / I  
G53 = (1-2) 164

HC—G30  
164

DER: or pharmaceutically acceptable salts or esters  
MPL: claim 1  
NTE: substitution is restricted  
STE: and racemates, diastereoisomers and optical isomers

L8 ANSWER 3 OF 8 MARPAT COPYRIGHT 2000 ACS

ACCESSION NUMBER: 130:168665 MARPAT  
TITLE: Preparation of hepatitis C inhibitory peptides  
INVENTOR(S): Llinas-Brunet, Montse; Poupart, Marc-Andre; Rancourt,  
Jean; Simoneau, Bruno; Tsantrizos, Youla; Wernic,  
Dominik  
PATENT ASSIGNEE(S): Boehringer Ingelheim (Canada) Ltd., Can.  
SOURCE: PCT Int. Appl., 158 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:



PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9907733	A2	19990218	WO 1998-CA765	19980810
WO 9907733	A3	19990520		
W:	AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
AU 9887956	A1	19990301	AU 1998-87956	19980810
EP 1003775	A2	20000531	EP 1998-939450	19980810
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI			

PRIORITY APPLN. INFO.:

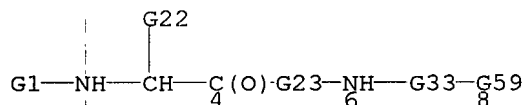
US 1997-55186 19970811

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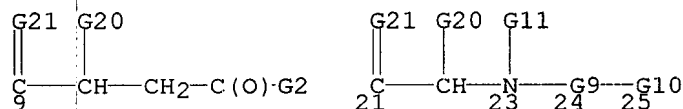
WO 1998-CA765 19980810

AB Peptides B[NHCHR6CO]a[NHCHR5CO]bQCHR4C(:Z)NHCHR3COWNHCR1R1'COA (when Q is CH2 and a and b are 0, B is an amide deriv. or when Q is NH or alkylimino and a and b are 0 or 1, B is an acyl deriv.; R6 = carboxyalkyl; R5 = alkyl or carboxyalkyl; R4 = alkyl, cycloalkyl, alkylcycloalkyl; Z = oxo or thioxo; R3 = alkyl, carboxyalkyl, cycloalkyl, alkylcycloalkyl; W is an amino acid residue such as proline; R1' = H and R1 = alkyl, mercapto- or haloalkyl or R1' and R1 together form a 3- to 6-membered ring; A is hydroxy or a pharmaceutically acceptable salt or ester) were prepd. as hepatitis C virus inhibitors. Thus, Ac-Asp-D-Glu-Chg-Val-X-Nva-OH [Chg = cyclohexylglycine, X = 4(R)-(2-naphthylmethoxy)proline, and Nva = norvaline residue], prepd. by step-wise couplings in soln., showed IC50 = 0.028 .mu.M in the NS3 protease/NS4A cofactor peptide radiometric assay.

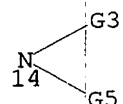
# MSTR 1



G1 = 9 / 21



G2 = 14 / Hy<EC (1-) Q (1-) N, AN (1-) N, RC (1), RS (1) X7> (SO G8) / (SC piperidino (SO G8))



G3 = H / alkyl<(1-10)> (SO G4) / cycloalkyl<(3-7)> (SO CO2H) / Ph / alkyl<(1-4)> (SR Ph) / alkyl<(1-6)> (SR cycloalkyl<(3-7)>) / alkyl<(1-6)> (SR Hy<EC (1-4) Q (0-) N (0-) O (0-) S (0) OTHERQ, RC (1), RS (1) M5 (1) X7>) / (SC 132 / Pr-i /

368866

CH2CH2CO2H / CH2CH2Ph / CH2Ph)

H<sub>2</sub>C—G40  
132

G4 = CO2H / dialkylamino<(1-6)>  
G5 = alkyl<(1-6)> (SR 17) /  
alkyl<(1-6)> (SR aryl<(6-10)> (SO G7)) / (SC CH2CH2CO2H /  
Ph (SO G54) / alkyl<(1-2)> (SR Ph (SO G54)))

C(O)-G6  
17

G6 = OH / alkoxy<(1-6)> / OCH2Ph  
G7 = 19 / alkyl<(1-6)> (SR Hy<EC (1-4) Q (0-) N (0-)  
O (0-) S (0) OTHERQ, RC (1), RS (1) M5 (1) X7>)

C(O)-G6  
19

G8 = CO2H / alkoxycarbonyl<(1-6)>  
G9 = NULL / 26-23 28-25 / 30-23 35-25

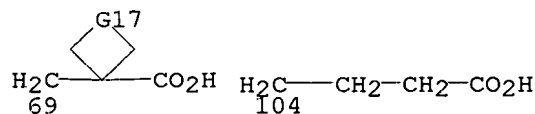
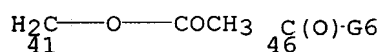
G18 G18 G19  
C(O)-CH-NH C(O)-CH-NH-C(O)-CH-NH  
26 28 30 35

G10 = 37 / 39

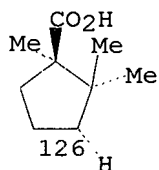
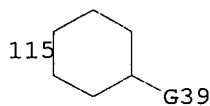
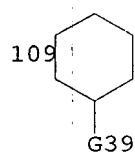
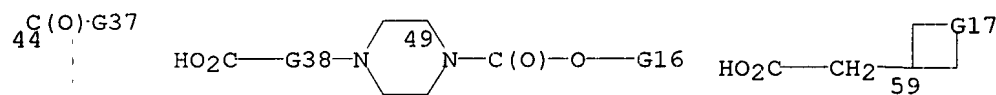
C(O)-G12 C(O)-G13  
37 39

G11 = H / alkyl<(1-6)> / (SC Me)  
G12 = alkyl<(1-10)> (SO G14) / 41 /  
alkyl<(1-7)> (SR cycloalkyl<(3-7)> (SO 46)) / 69 /  
alkyl<(1-6)> (SR aryl<(6-10)> (SO alkyl<(1-6)>)) /  
(SC CH2CH2CO2H / 104 / Me / CH2Ph / CH2CH2Ph)

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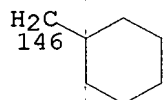


G13 = cycloalkyl<(3-7)> (SO 44) /  
 cycloalkyl<(3-7)> (SR (2-4) G15) / 49 / 59 /  
 aryl<(6-10)> (SO alkyl<(1-6)>) / (SC OBU-t / 109 / 115 /  
 126 / cyclopentyl (SO CO2H) / cyclohexyl (SO CO2H) / Ph)

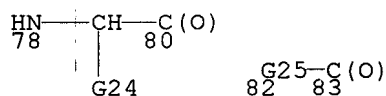


G14 = CO2H / OCHO / alkylcarbonyloxy<(1-5)> /  
 alkoxy<(1-6)> / (SC OCOMe / OMe / OEt / OPr-n / OBU-t)  
 G15 = (1) CO2H / (1-3) alkyl<(1-6)>  
 G16 = aryl / alkyl<(1-6)> (SR aryl) / (SC CH2Ph)  
 G17 = (0-4) CH2  
 G18 = alkyl<(1-6)> (SO CO2H) / (SC CH2CO2H / CH2CH2CO2H /  
 Pr-i / Bu-t)  
 G19 = alkyl<(1-6)> (SR CO2H) / (SC CH2CO2H / CH2CH2CO2H)  
 G20 = alkyl<(1-10)> / cycloalkyl<(3-7)> /  
 alkyl<(1-7)> (SR cycloalkyl<(3-7)>) / (SC Pr-i /  
 cyclopropyl / Bu-t / Bu-s / Bu-i / cyclohexyl)  
 G21 = O / S  
 G22 = **alkyl<(1-10)> (SO CO2H) / cycloalkyl<(3-7)> /**  
 alkyl<(1-7)> (SR cycloalkyl<(3-7)>) / (SC Bu-s / cyclohexyl /  
 146 / Pr-i / Bu-t / CH2CH2CO2H / H)

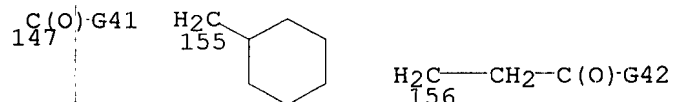
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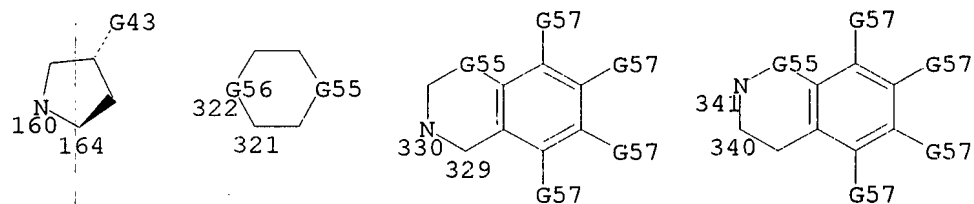
G23 = 78-4 80-6 / **82-4 83-6**



G24 = alkyl<(1-10)> (SO CO2H) /  
cycloalkyl<(3-10)> (SO CO2H) / aryl<(6-10)> /  
alkyl<(1-6)> (SR aryl<(6-10)>) / (SC alkyl<(1-6)> (SR 147) /  
CH2Ph / Et / Bu-i / 155 / Pr-i / Me / CH2CO2H / 156)

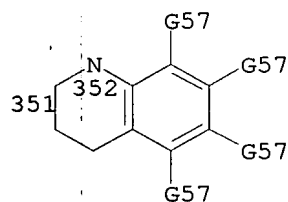


G25 = Cy<EC (5-6) A (0-) Q (0-) N (4-) C,  
AN (0-) N (1-) C, RC (1-2), RS (0-) E5 (0-) E6 (-1) E7 (0)  
OTHER> (SO (1-) G26) / (**sc 160-4 164-83** / 322-4 321-83 /  
330-4 329-83 / 341-4 340-83 / 352-4 351-83 )





368866



G26 = OH / SH / NH<sub>2</sub> / CO<sub>2</sub>H / cycloalkyl<(3-16)> (SO) /  
alkyl<(1-16)> (SO) / cycloalkenyl<(3-16)> (SO) /  
alkenyl<(2-16)> (SO) / Hy<EC (1-) Q (0-) N (0-) O (0-) S (0)  
OTHERQ, AR (0), BD (0-) D (0) T> (SO) / 84 / 89 / 93 /  
aryl<(6-10)> (SO) / alkyl<(1-6)> (SR G32) /  
heteroaryl<EC (1-) Q (0-) N (0-) O (0-) S (0-) OTHERQ> (SO)

<sup>84</sup>G27-G28-G27 <sup>89</sup>G31-G30 <sup>93</sup>C(O)O—G30

G27 = Ak<EC (1-16) C, BD (0-) D (0) T> (SO)  
G28 = O / S / 87

<sup>87</sup>N—G29

G29 = H / Ak<EC (1-16) C, BD (0-) D (0) T> (SO)  
G30 = cycloalkyl<(3-16)> (SO) / alkyl<(1-16)> (SO) /  
cycloalkenyl<(3-16)> (SO) / alkenyl<(2-16)> (SO) /  
Hy<EC (1-) Q (0-) N (0-) O (0-) S (0) OTHERQ, AR (0),  
BD (0-) D (0) T> (SO) / 96 / aryl<(6-10)> (SO) /  
alkyl<(1-6)> (SR G32) / heteroaryl<EC (1-) Q (0-) N (0-)  
O (0-) S (0-) OTHERQ> (SO)

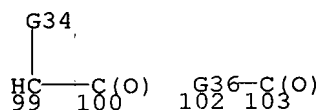
<sup>96</sup>G27-G28-G27

G31 = O / S / NH / 91

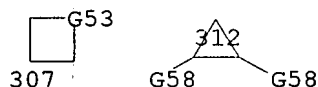
<sup>91</sup>N—G30

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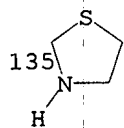
G32 = aryl<(6-10)> (SO) / heteroaryl<EC (1-) Q (0-) N (0-)  
O (0-) S (0-) OTHERQ> (SO)  
G33 = 99-6 100-8 / **102-6 103-8**



G34 = alkyl<(1-6)> (SO (1-) G35) / alkenyl<(2-6)> /  
(SC CH2SH / Et / Pr-n / CH2CH=CH2 / Me / Pr-i / CH2CH2SMe)  
G35 = SH / F / Cl / Br / I  
G36 = cycloalkylene<(3-6)> (SO alkyl<(1-6)>) / (SC 307 /  
**312**)

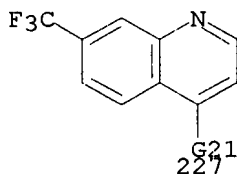
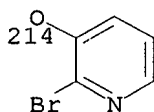
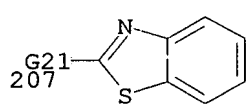
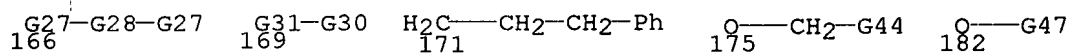


G37 = OH / alkoxy<(1-6)> / OCH2Ph / (SC OMe / OEt)  
G38 = alkylene<(1-6)> / (SC CH2)  
G39 = CO2H / CO2CH2Ph  
G40 = 2-tetrahydrofuryl / 135 / cyclopropyl / 2-thienyl

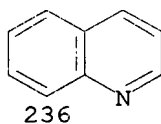
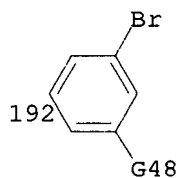
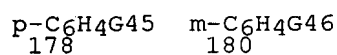


G41 = OH / alkoxy<(1-6)> / OCH2Ph / NHCH2Ph  
G42 = OH / OCH2Ph / NHCH2Ph  
G43 = OH / SH / NH2 / **CO2H** / cycloalkyl<(3-16)> (SO) /  
alkyl<(1-16)> (SO) / cycloalkenyl<(3-16)> (SO) /  
alkenyl<(2-16)> (SO) / Hy<EC (1-) Q (0-) N (0-) O (0-) S (0)  
OTHERQ, AR (0), BD (0-) D (0) T> (SO) / 166 / 169 /  
aryl<(6-10)> (SO) / alkyl<(1-6)> (SR G32) /  
heteroaryl<EC (1-) Q (0-) N (0-) O (0-) S (0-) OTHERQ> (SO) /  
CH2Ph / CH2CH2Ph / 171 / 175 / 182 / 207 / 214 / 227

368866



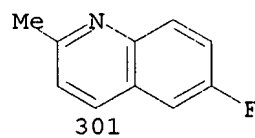
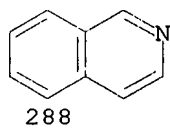
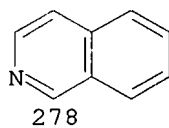
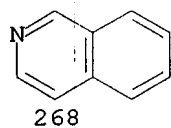
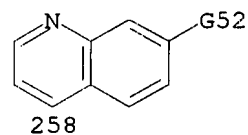
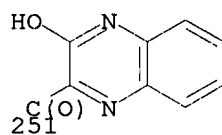
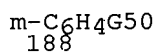
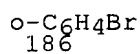
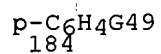
G44 = 178 / o-C<sub>6</sub>H<sub>4</sub>Me / 180 / naphthyl / 192 / 236



G45 = H / Me / Bu-t

G46 = Me / I

G47 = naphthyl / 184 / 186 / 188 / 251 / 258 / 268 / 278 / 288 / 301



G48 = H / Br

368866

G49 = Br / I / 228

p-C<sub>6</sub>H<sub>4</sub>OMe  
228

G50 = Br / 292

m-C<sub>6</sub>H<sub>4</sub>G51  
292

G51 = H / NHCOMe / CH<sub>2</sub>OH / NO<sub>2</sub>  
G52 = H / Cl  
G53 = (1-3) CH<sub>2</sub>  
G54 = CO<sub>2</sub>H / alkoxycarbonyl<(1-4)>  
G55 = (0-1) CH<sub>2</sub>  
G56 = N / CH  
G57 = H / 365

O—G55—CH<sub>2</sub>—Ph  
365

G58 = H / alkyl<(1-6)> / Et  
G59 = OH / (SC alkoxy<(1-6)> (SO aryl) / OMe / OEt / OPh /  
OCH<sub>2</sub>Ph)  
DER: or pharmaceutically acceptable salts or esters  
MPL: claim 1  
NTE: additional ring formation also claimed  
NTE: also incorporates broader disclosure  
NTE: substitution is restricted

L8 ANSWER 4 OF 8 MARPAT COPYRIGHT 2000 ACS

(ALL HITS ARE ITERATION INCOMPLETES)

ACCESSION NUMBER: 131:179820 MARPAT

TITLE: Pharmaceutical compositions of guanidine derivatives  
for the treatment of ischemic brain damage

INVENTOR(S): Kuribayashi, Yoshikazu; Itoh, Natsuko; Ohashi,  
Naohito

PATENT ASSIGNEE(S): Sumitomo Pharmaceuticals Co., Ltd., Japan

SOURCE: Eur. Pat. Appl., 28 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

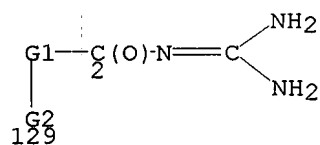
FAMILY ACC. NUM. COUNT: 1

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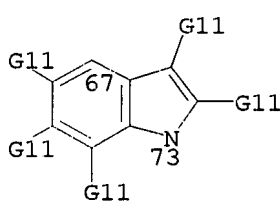
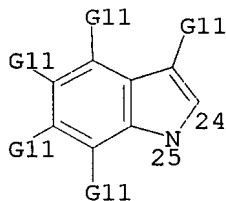
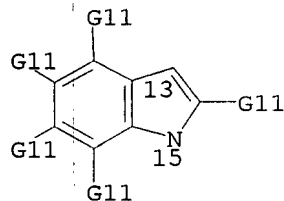
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 937459	A2	19990825	EP 1999-300678	19990129
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 11286454	A2	19991019	JP 1999-12055	19990120
PRIORITY APPLN. INFO.:			JP 1998-34110	19980129
AB The use of a guanidine compd. which has Na <sup>+</sup> /H <sup>+</sup> exchange system inhibition activity, or a pharmaceutically acceptable acid addn. salt thereof, in the				
manuf. of a pharmaceutical compn. for the treatment of ischemic brain damage such as cerebral infarction, cerebral embolism and cerebral thrombus is described. E.g., the mean percentage of the infarcted area of				
brain sections in rats given 1,4-dimethyl-2-indoloylguanidine methanesulfonate (1 mg/mL/kg i.p.) 30 min before the occlusion of the middle cerebral artery was 26.6 .+- 3.1% compared to 49.5 .+- 4.1% in the control vehicle-treated animals.				

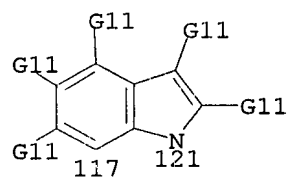
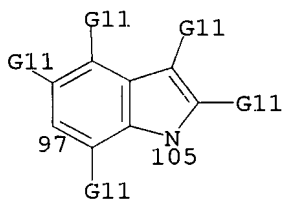
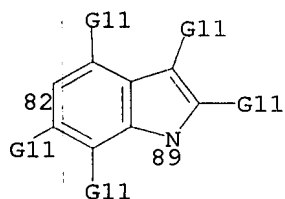
MSTR 1 ITERATION INCOMPLETE



G1 = 13-2 15-129 / 24-2 25-129 / 67-2 73-129 /  
82-2 89-129 / 97-2 105-129 / 117-2 121-129



368866



G2 = H / alkyl<(1-8)> (SO (1-) G3) / cycloalkyl<(3-7)> /  
OH / alkoxy<(1-6)> / aryl<(-10)> (SO) /  
heteroaryl<EC (0-4) N (-1) O (-1) S> (SO) / 26 / (SC Me)

H<sub>2</sub>C—G4  
26

G3 = X / OH / alkoxy<(1-6)> / CN / CO<sub>2</sub>H /  
alkoxycarbonyl<(1-6)> / alkylcarbonyl<(1-8)> (SO aryl<(6-)>  
) / arylcarbonyl<(6-10)> / aryl<(-10)> (SO) /  
heteroaryl<EC (0-4) N (-1) O (-1) S> (SO) / 30 / NH<sub>2</sub> / 32 /  
Hy<EC (1-) Q (1-) N, AN (1-) N, AR (0), BD (ALL) SE,  
RS (0-) E5 (0-) E6 (0-) E7 (0) OTHER> (SO) / 40

C(=O)—G5    G6—G7    G8—G9  
30            32            40

G4 = alkenyl<(2-6)> / alkynyl<(2-6)>  
G5 = NH<sub>2</sub> / alkylamino<(1-8)> / dialkylamino<(1-8)> /  
Hy<EC (1-) Q (1-) N, AN (1-) N, AR (0), BD (ALL) SE,  
RS (0-) E5 (0-) E6 (0-) E7 (0) OTHER> (SO)  
G6 = NH / 34

N—G7  
34

G7 = alkyl<(1-8)> (SO) / cycloalkyl<(3-7)> /  
alkylcarbonyl<(1-8)> (SO aryl<(6-)>) / arylcarbonyl<(6-10)> /  
aryl<(-10)> (SO) / heteroaryl<EC (0-4) N (-1) O (-1) S>  
(SO) / 36

368866

H<sub>2</sub>C—G4  
36

G8 = cycloalkylene<(3-8)> /  
Hy<EC (2-7) C (1) Q (1) N (0) OTHERQ, AN (1) C (1) N,  
AR (0), BD (ALL) SE, RC (1), RS (1) M3 (1) X8>  
G9 = H / alkyl<(1-8)> (SO (1-) G10)  
G10 = OH / alkoxy<(1-6)> / CN / CO<sub>2</sub>H /  
alkoxycarbonyl<(1-6)> / alkylcarbonyl<(1-8)> (SO aryl<(6-)>  
) / arylcarbonyl<(6-10)> / aryl<(-10)> (SO) /  
heteroaryl<EC (0-4) N (-1) O (-1) S> (SO) / 42 / NH<sub>2</sub> / 130 /  
Hy<EC (1-) Q (1-) N, AN (1-) N, AR (0), BD (ALL) SE,  
RS (0-) E5 (0-) E6 (0-) E7 (0) OTHER> (SO) / 132

C(O)·G5    G<sub>6</sub>—G7    C(O)·G5  
42    130    132

G11 = H / alkyl<(1-8)> / alkenyl<(2-6)> / alkynyl<(2-6)> /  
cycloalkyl<(3-7)> / X / NO<sub>2</sub> / alkylcarbonyl<(1-8)>  
(SO aryl<(6-)>) / arylcarbonyl<(6-10)> / CO<sub>2</sub>H /  
alkoxycarbonyl<(1-6)> / aryl<(-10)> (SO) /  
heteroaryl<EC (0-4) N (-1) O (-1) S> (SO) / OH / 54 /  
NH<sub>2</sub> (SO) / SO<sub>2</sub>NH<sub>2</sub> (SO) / 56 / 58

O—G18    G<sub>12</sub>—G13    G<sub>14</sub>—G15—G16  
54    56    58

G12 = S / S(O) / SO<sub>2</sub>  
G13 = alkyl<(1-8)> (SO) / aryl<(-10)> (SO) /  
heteroaryl<EC (0-4) N (-1) O (-1) S> (SO)  
G14 = O / S / S(O) / SO<sub>2</sub> / NH / 61

N—G17  
61

G15 = Hy<EC (2-7) C (1) Q (1) N (0) OTHERQ,  
AN (1) C (1) N, AR (0), BD (ALL) SE, RC (1),  
RS (1) M3 (1) X8>  
G16 = H / alkyl<(1-8)> (SO)  
G17 = alkyl<(1-8)>

368866

G18 = alkyl<(1-8)> (SO) / cycloalkyl<(3-7)> /  
alkylcarbonyl<(1-8)> (SO aryl<(6-)>) / arylcarbonyl<(6-10)> /  
aryl<(-10)> (SO) / heteroaryl<EC (0-4) N (-1) O (-1) S>  
(SO) / 63

H<sub>2</sub>C—G4  
63

DER: or pharmaceutically acceptable acid addition salts  
MPL: claim 3

L8 ANSWER 5 OF 8 MARPAT COPYRIGHT 2000 ACS

(ALL HITS ARE ITERATION INCOMPLETES)

ACCESSION NUMBER: 125:247472 MARPAT

TITLE: Substituted styryl heterocyclic amido prostaglandin  
analogs

INVENTOR(S): Misra, Raj N.

PATENT ASSIGNEE(S): E.R. Squibb and Sons, Inc., USA

SOURCE: U.S., 14 pp.

CODEN: USXXAM

DOCUMENT TYPE: Patent

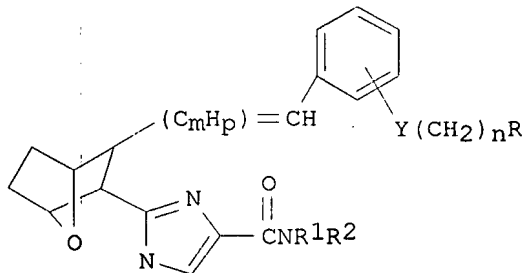
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5550248	A	19960827	US 1990-619569	19901129

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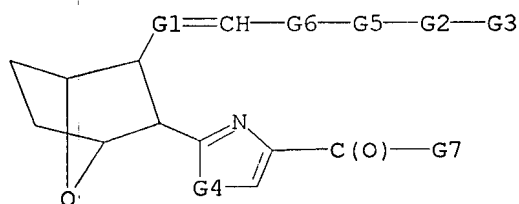
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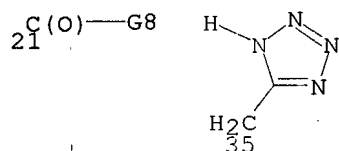
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AB Prostaglandin analogs useful in treating thrombotic and vasospastic disease having the structural formula I wherein: CmHp is an alkylene chain wherein m is 0, 1, 2, or 3 and p=(2.times.m)-1, except that when m is 0, p is also 0; n is 0, 1, 2 or 3; R is CO2R', CH2OH, CONHSO2R3, CONHR4, or -CH2-(5-tetrazolyl); R' is hydrogen, alkyl, or alkali metal; X is O or NH; Y is --O--, a single bond or vinylene, except that Y cannot be --O-- when n is 0; and the remaining symbols are as defined in the specification.

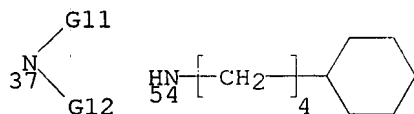
**MSTR 1 ITERATION INCOMPLETE**



G1 = NULL / Ak<EC (1-3) C, BD (ALL) S> / (EX CH)  
 G2 = (0-3) CH2  
 G3 = 21 / CH2OH / 35



G4 = O / NH  
 G5 = O / NULL / CH=CH  
 G6 = phenylene  
 G7 = 37 / Hy<EC (1) Q (1) N, AN (1) N, RC (1), RS (1) M5 (1) X8> / (SC 54)



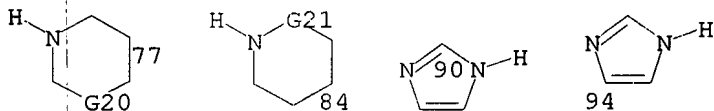
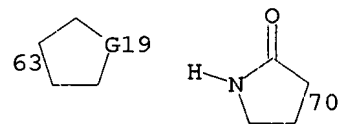
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G8 = OH / alkoxy<(1-12)> / 22 / 24 / NH2 /  
alkylamino<(1-12)> / arylamino<(6-12)> / aralkylamino

OH  
22 ● G9 HN—SO<sub>2</sub>—G10  
24

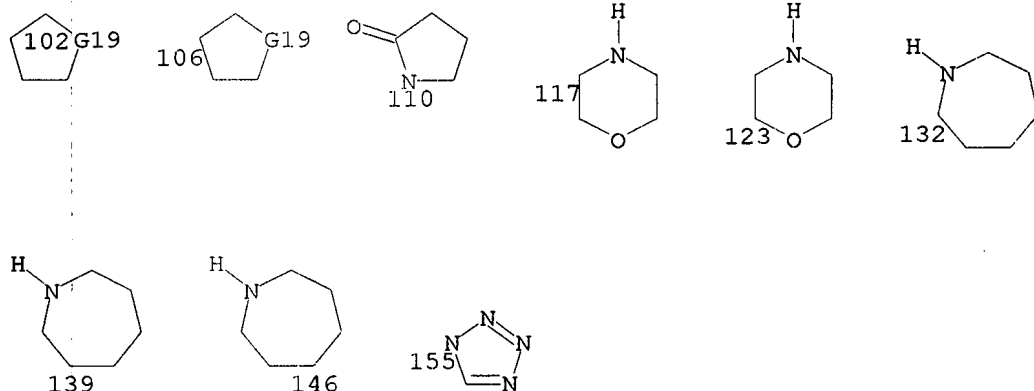
G9 = alkali metal atom  
G10 = alkyl<(1-12)> / aryl<(6-10)> / aralkyl  
G11 = H / alkyl<(1-12)> (SO G17) /  
alkenyl<(-12)> (SO G17) / alkynyl<(-16)> (SO G17) /  
aralkyl (SO G17) / aryl<(6-10)> (SO G17) /  
cycloalkyl<(3-12)> (SO G17) / 40 /  
Hy<EC (1-2) Q (0-) N (0-) O (0-) S (0) OTHERQ, AN (1-) C,  
RC (1), RS (1) M5 (1) X7> (SO G17) /  
heteroaryl<AN (1-) C> (SO G17) / 42 / 46 / (EX 63 / 70 / 77 /  
84 / pyridyl / pyrimidinyl / oxazolyl / thiazolyl / 90 / 94)

G13—G14 G15—C(O)—NH—G16 G15—NH—C(O)—G16  
40 42 46



G12 = H / alkyl<(1-12)> / aryl<(6-10)> / aralkyl /  
(EX CH2Ph)  
G13 = (1-12) CH2  
G14 = cycloalkyl<(3-12)> (SO G17) /  
Hy<EC (1-2) Q (0-) N (0-) O (0-) S (0) OTHERQ, RC (1),  
RS (1) M5 (1) X7> (SO G17) / heteroaryl<AN (1-) C> (SO G17) /  
(EX 102 / 106 / pyrrolyl / piperidino / 110 / 117 / 123 /  
morpholino / thiomorpholino / 132 / 139 / 146 /  
hexahydroazepino / pyrazinyl / imidazolyl / pyrimidinyl /  
oxazolyl / thiazolyl / 155 / pyridyl)

368866



G15 = (1-12) CH2  
 G16 = alkyl<(1-12)> (SO G17) / aryl<(6-10)> (SO G17) /  
 cycloalkyl<(3-12)> (SO G17) / 50

G13-G18  
 50

G17 = alkyl<(1-12)> / aryl<(6-10)> / cycloalkyl<(3-12)> /  
 52

G13-G18  
 52

G18 = cycloalkyl<(3-12)> (SO)  
 G19 = O / S  
 G20 = CH2 / CH2CH2  
 G21 = CH2 / CH2CH2  
 DER: and pharmaceutically acceptable salts  
 MPL: claim 1  
 NTE: if G2 = (0)CH2, then not G5 = O

L8 ANSWER 6 OF 8 MARPAT COPYRIGHT 2000 ACS  
 (ALL HITS ARE ITERATION INCOMPLETES)

ACCESSION NUMBER: 121:109397 MARPAT

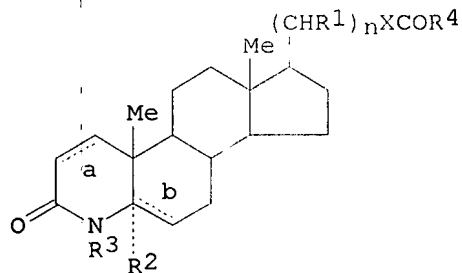
TITLE: Preparation of ester derivatives of 4-azasteroids as  
 steroid 5.alpha.-reductase inhibitors.

368866

INVENTOR(S): Witzel, Bruce E.; Rasmusson, Gary H.; Tolman, Richard L.; Yang, Shu Shu  
 PATENT ASSIGNEE(S): Merck and Co., Inc., USA  
 SOURCE: PCT Int. Appl., 66 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 2  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9323041	A1	19931125	WO 1993-US4771	19930519
W: AU, BB, BG, BR, CA, CZ, FI, HU, JP, KR, KZ, LK, MG, MN, MW, NO, NZ, PL, RO, RU, SD, SK, UA, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9342525	A1	19931213	AU 1993-42525	19930519
AU 668181	B2	19960426		
EP 649306	A1	19950426	EP 1993-911362	19930519
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
JP 07508039	T2	19950907	JP 1993-503838	19930519
US 5610162	A	19970311	US 1994-338573	19941117
PRIORITY APPLN. INFO.:				US 1992-886022 19920520
				WO 1993-US4771 19930519

GI

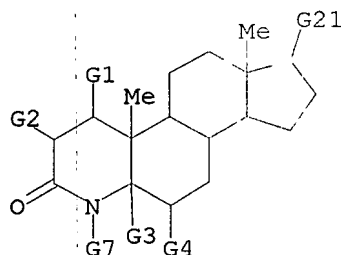


AB Title compds. [I; a, b = single bonds, R2 = H; or a = single bond, b = double bond, and R2 = null; R1 = H, aryl, alkyl, aralkyl; R3 = H, Me, Et, OH, NH2, SMe; n = 0-10; X = O, S; R4 = (substituted) alkyl, aryl, heterocyclyl, cycloalkyl, amino, OH, etc.] were prep'd. as inhibitors of 5.alpha.-reductase and isoenzymes thereof. The compds. are useful for the

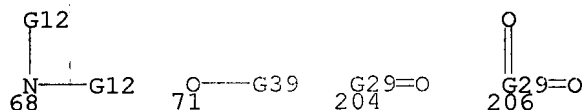
368866

treatment of hyperandrogenic disease conditions and diseases of the skin and scalp (no data). Thus, 20-hydroxy-4-methyl-5.alpha.-4-azapregnan-3-one, 11-ethylthioundecanoic acid, DMAP, and DCC were stirred in CH<sub>2</sub>Cl<sub>2</sub> at room temp. to give 20-[11-(ethylthio)undecanoyloxy]-4-methyl-5.alpha.-4-azapregnan-3-one.

**MSTR 1 ITERATION INCOMPLETE**



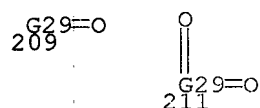
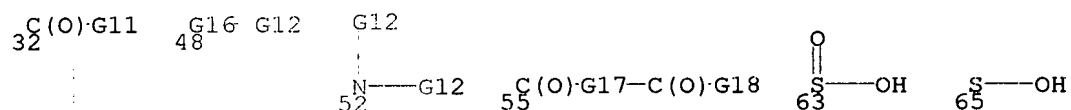
G1 = H  
 G2 = H  
 G3 = H  
 G4 = H  
 G5 = NULL / alkylene<EC (1-10) C, DC (0) M3> (SO G6)  
 G6 = Ph / naphthyl / alkyl<(1-3)> (SO G28) / (SC Me)  
 G7 = H / Me / Et / OH / NH<sub>2</sub> / SMe  
 G8 = O / S  
 G9 = Ph (SO) / naphthyl (SO) /  
 Hy<EC (1-3) Q (0-) N (0-) O (0-) S (0) OTHERQ, CH (-1) +,  
 RC (1), RS (1) M5 (1) X7> (SO) / 204 / 206 /  
 Hy<EC (1-3) Q (0-) N (0-) O (0-) S (0) OTHERQ (6) C,  
 AR (1-), BD (6-) N, CH (-1) +, RC (2),  
 RS (0-) E5 (1-) E6 (0-) E7 (0) OTHER> (SO) /  
 cycloalkyl<(3-10)> (SO) / 68 / OH / 71



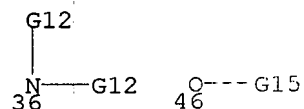
G10 = OH / F / Cl / Br / I / alkoxy<(1-8)> /  
 alkenyl<(1-6)> / 32 / SH / 65 / 63 / 48 / 52 / Ph (SO) /  
 naphthyl (SO) / Hy<EC (1-3) Q (0-) N (0-) O (0-) S (0)  
 OTHERQ, CH (-1) +, RC (1), RS (1) M5 (1) X7> (SO) / 209 /  
 211 / Hy<EC (1-3) Q (0-) N (0-) O (0-) S (0) OTHERQ (6) C,

368866

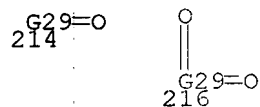
AR (1-), BD (6-) N, CH (-1) +, RC (2),  
RS (0-) E5 (1-) E6 (0-) E7 (0) OTHER> (SO) /  
cycloalkyl<(3-10)> (SO) / 55



G11 = 36 / OH / 46

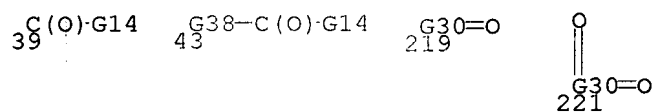


G12 = H / alkyl<(1-8)> (SO (1-) G13) / Ph (SO) /  
naphthyl (SO) / Hy<EC (1-3) Q (0-) N (0-) O (0-) S (0)  
OTHERQ, CH (-1) +, RC (1), RS (1) M5 (1) X7> (SO) / 214 /  
216 / Hy<EC (1-3) Q (0-) N (0-) O (0-) S (0) OTHERQ (6) C,  
AR (1-), BD (6-) N, CH (-1) +, RC (2),  
RS (0-) E5 (1-) E6 (0-) E7 (0) OTHER> (SO)

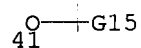


G13 = OH / alkoxy<(1-3)> / CN / 39 / 43 / NO2 / F / Cl /  
Br / I / NH2 / alkylamino<(1-4)> / dialkylamino<(1-4)> /  
Ph (SO) / naphthyl (SO) / Hy<EC (1-3) Q (0-) N (0-) O (0-)  
S (0) OTHERQ, CH (-1) +, RC (1), RS (1) M5 (1) X7> / 219 /  
221 / Hy<EC (1-3) Q (0-) N (0-) O (0-) S (0) OTHERQ (6) C,  
AR (1-), BD (6-) N, CH (-1) +, RC (2),  
RS (0-) E5 (1-) E6 (0-) E7 (0) OTHER>

368866



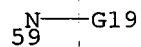
G14 = OH / 41



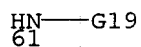
G15 = alkyl<(1-8)> (SO) / Ph (SO) / naphthyl (SO)

G16 = S / S(O) / SO2

G17 = NH / 59

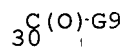


G18 = NH2 / 61

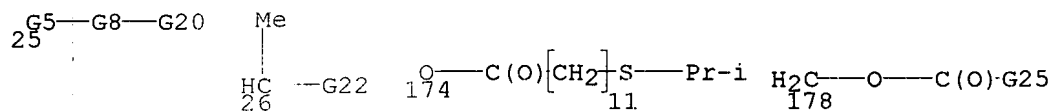


G19 = alkyl<(1-8)> / CH2Ph / cyclohexyl

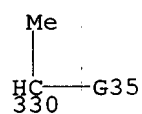
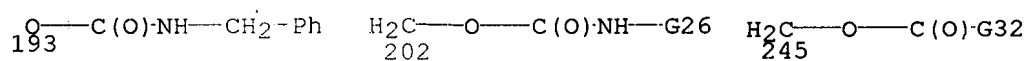
G20 = alkylcarbonyl<(1-20)> (SO (1-) G10) / 30



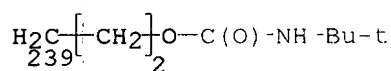
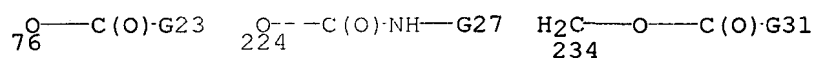
G21 = 25 / (SC 26 / 174 / 178 / 193 / 202) / (EX 245 / 330)



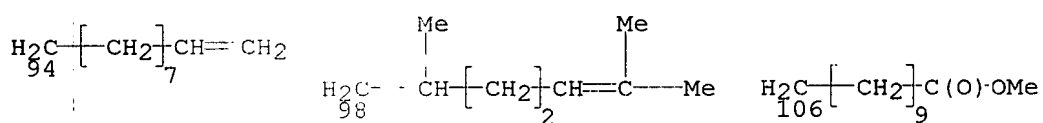
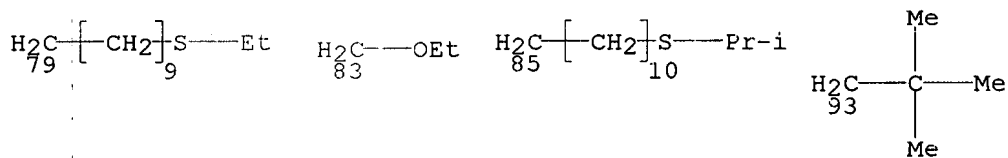
368866



G22 = 76 / 224 / 234 / 239

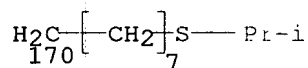
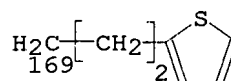
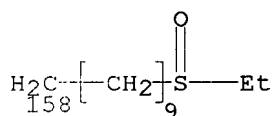
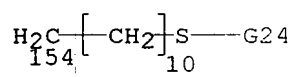
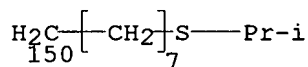
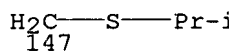
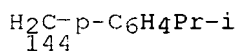
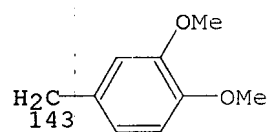
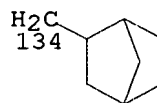
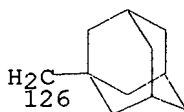
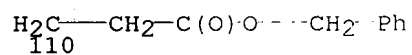


G23 = 79 / 83 / 85 / dodecyl / 93 / Bu-t / 94 / 98 /  
CH<sub>2</sub>CH<sub>2</sub>CO<sub>2</sub>H / 106 / 110 / 126 / 134 / 143 / 144 / 147 / 150 /  
154 / 158 / 169 / 170



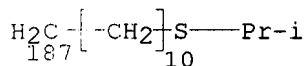
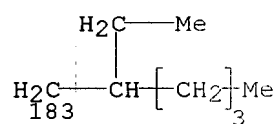


368866



G24 = Pr-i / Bu-t

G25 = Me / Bu-t / 183 / 187



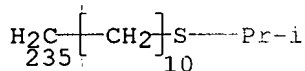
G26 = Bu-t / Me / 228

o-C<sub>6</sub>H<sub>4</sub>Et  
228

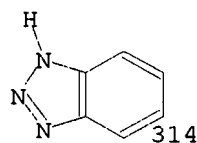
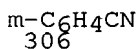
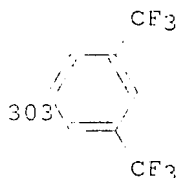
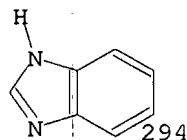
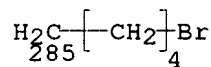
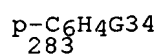
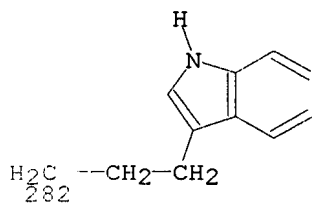
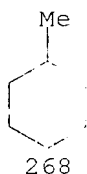
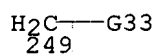
G27 = Bu-t / Pr-i / Me

368866

G28 = Ph / naphthyl  
 G29 = Hy<EC (1-3) Q (0-) N (0-) O (0-) S (0) OTHERQ,  
 AN (0-) N (0-) S (0) OTHERQ, CH (-1) +, RC (1),  
 RS (1) M5 (1) X7> (SO) / Hy<EC (1-3) Q (0-) N (0-) O (0-)  
 S (0) OTHERQ (6-) C, AR (1-), BD (6-) N, CH (-1) +, RC (2),  
 RS (0-) E5 (1-) E6 (0-) E7 (0) OTHER> (SO)  
 G30 = Hy<EC (1-3) Q (0-) N (0-) O (0-) S (0) OTHERQ,  
 AN (0-) N (0-) S (0) OTHERQ, CH (-1) +, RC (1),  
 RS (1) M5 (1) X7> / Hy<EC (1-3) Q (0-) N (0-) O (0-) S (0)  
 OTHERQ (6-) C, AR (1-), BD (6-) N, CH (-1) +, RC (2),  
 RS (0-) E5 (1-) E6 (0-) E7 (0) OTHER>  
 G31 = Me / Bu-t / 235

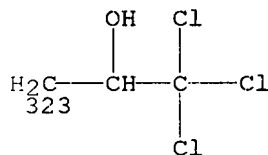


G32 = 249 / 268 / 282 / 283 / 285 / 294 / 303 / 306 /  
 314 / 320 / 323 / CH=CHPh



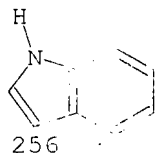
368866

i-Pr-p-C<sub>6</sub>H<sub>4</sub>CH<sub>3</sub>p-C<sub>6</sub>H<sub>4</sub>Pr-i  
320



G33 = 2-furyl / 251 / cyclohexyl / 256 / OCOME

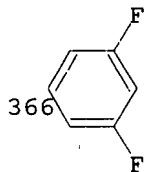
p-C<sub>6</sub>H<sub>4</sub>Pr-i  
251



G34 = Bu-i / OEt

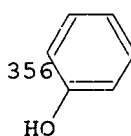
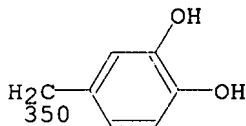
G35 = 333 / 358 / heptadecyl / 366

H<sub>2</sub>C-O-C(O)G36 p-C<sub>6</sub>H<sub>4</sub>NH-COCH<sub>3</sub>  
333 358



G36 = 337 / pentadecyl / 339 / 350 / 356

p-C<sub>6</sub>H<sub>4</sub>G37 F<sub>2</sub>C-CF<sub>2</sub>-CF<sub>3</sub>  
337 339

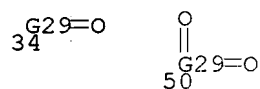


G37 = NO<sub>2</sub> / CPh

G38 = alkylene<(1-8)>

G39 = H / alkyl<(1-8)> (SO (1-) G13) / Ph (SO) /  
naphthyl (SO) / Hy<EC (1-3) Q (0-) N (0-) O (0-) S (0)  
OTHERQ, CH (-1) +, RC (1), RS (1) M5 (1) X7> (SO) / 34 / 50 /  
Hy<EC (1-3) Q (0-) N (0-) O (0-) S (0) OTHERQ (6) C,  
AR (1-), BD (6-) N, CH (-1) +, RC (2),  
RS (0-) E5 (1-) E6 (0-) E7 (0) OTHER> (SO)

368866



G1 +G2 = NULL

G3 +G4 = NULL

DER: or pharmaceutically acceptable salts or ester

MPL: claim 1

L8 ANSWER 7 OF 8 MARPAT COPYRIGHT 2000 ACS

(ALL HITS ARE ITERATION INCOMPLETES)

ACCESSION NUMBER: 120:245602 MARPAT

TITLE: Preparation of 17-ethers and thioethers of  
4-aza-steroids as steroid reductase inhibitors

INVENTOR(S): Witzel, Bruce E.; Tolman, Richard L.; Rasmusson, Gary  
H.; Bakshi, Raman K.; Yang, Shu Shu

PATENT ASSIGNEE(S): Merck and Co., Inc., USA

SOURCE: PCT Int. Appl., 68 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

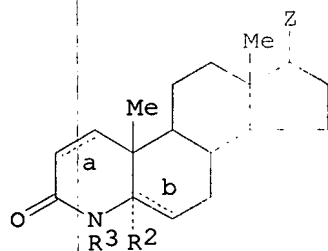
FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9323040	A1	19931125	WO 1993-US4746	19930519
W: AU, BB, BG, BR, CA, CZ, FI, HU, JP, KR, KZ, LK, MG, MN, MW, NO, NZ, PL, RO, RU, SD, SK, UA, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9342521	A1	19931213	AU 1993-42521	19930519
AU 668180	B2	19960426		
EP 641204	A1	19950308	EP 1993-911358	19930519
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
JP 07508038	T2	19950907	JP 1993-503831	19930519
US 5536727	A	19960716	US 1994-338572	19941117
PRIORITY APPLN. INFO.:			US 1992-886031	19920520
			WO 1993-US4746	19930519

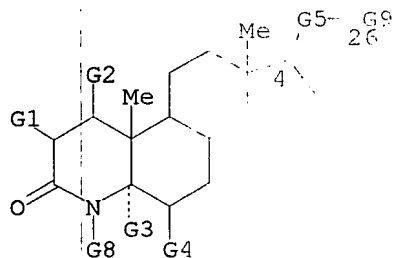
GI

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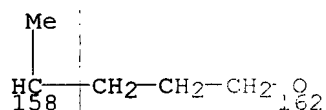
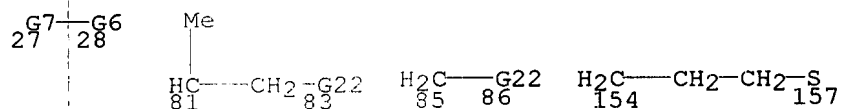
AB Title compds. [I; a, b both = single bonds, and R2 = H; or a = double bond, b = single bond, and R2 = H; or a = single bond, b = double bond, and R2 = null; R1 = H, aryl, (aryl)alkyl; R3 = H, Me, Et, OH, NH2, SMe; R4 = (substituted) alkyl, aryl, heterocyclyl; Z = XR4, (CHR1)nXR4; X = O, S, SO, SO2], were prepd. as inhibitors of steroid 5.alpha.-reductase enzymes 1 and 2 (no data). The compds. are useful for the treatment of hyperandrogenic disease conditions and diseases of the skin and scalp. Thus, 17-hydroxymethyl-4-methyl-5.alpha.-4-azaandrostan-3-one and diphenyldiazomethane in CH2Cl2 were treated dropwise with BF3.Et2O to give 17-diphenylmethoxymethyl-4-methyl-5.alpha.-4-azaandrostan-3-one.

MSTR 1 ITERATION INCOMPLETE

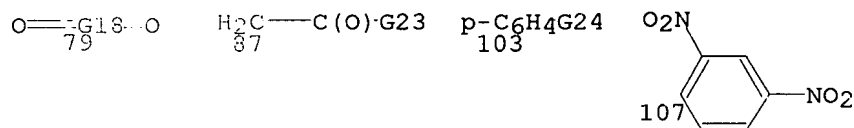
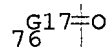



G1 = H  
G2 = H  
G3 = H  
G4 = H  
G5 = O / S / S(O) / SO2 / 27-4 28-26 / (SC 81-4 83-26 / 85-4 86-26 / 154-4 157-26 / 158-4 162-26 )

368866



G6 = O / S / S(O) / SO2  
 G7 = alkylene (SO G11)  
 G8 = H / Me / Et / OH / NH2 / SMe  
 G9 = alkyl<(1-20)> (SO (1-) G10) / Ph (SO) /  
 naphthyl (SO) / Hy<EC (1-3) Q (0-) N (0-) O (0-) S (0)  
 OTHERQ, RC (1), RS (1) M5 (1) X7> (SO) / 76 / 79 /  
 Hy<EC (1-3) Q (0-) N (0-) O (0-) S (0) OTHERQ (6-) C,  
 AR (1-), BD (0-) N, RC (2), RS (0-) E5 (1-) E6 (0-) E7 (0)  
 OTHER> (SO) / cycloalkyl<(3-10)> (SO) / (SC Me / 87 / Et /  
 CHPh2 / Pr-i / 103 / 107 / 119 / 3-pyridyl / 130 / 142 /  
 143 / hexyl / Pr-n / undecyl / CH2CH=CH2 / CH2CH2CHMe2 /  
 CH2C(Me)=CH2 / 168 / 170)



$$\begin{array}{c} \text{H}_2\text{C}-\text{C}(\text{O})-\text{N}-\text{C}(\text{O})\text{NH} \\ \text{119} \end{array}$$


$$\begin{array}{c} \text{H}_2\text{C}-\text{G25} \\ \text{130} \end{array} \quad \begin{array}{c} \text{H}_2\text{C}-\text{C}(\text{O})-\text{N}-\text{C}(\text{O})\text{NH}-\text{Pr-i} \\ \text{142} \end{array}$$

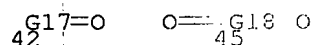
$$\begin{array}{ccccccc} \text{H}_2\text{C} & \text{---} & \text{CH}_2 & \text{---} & \text{CH} & & \text{Me} \\ 143 & & & & & & \end{array} \quad \begin{array}{cc} \text{o-C}_6\text{H}_4\text{G29} & \text{m-C}_6\text{H}_4\text{G30} \\ 168 & 170 \end{array}$$

$\begin{array}{c} \text{G12} \\ \diagup \\ \text{C(O)-N} \\ \diagdown \\ \text{G12} \end{array}$ 
 $\begin{array}{c} \text{C(O)-O} \\ \text{G14} \end{array}$ 
 $\begin{array}{c} \text{S-OH} \\ \text{50} \end{array}$ 
 $\begin{array}{c} \text{O} \\ \parallel \\ \text{S-OH} \\ \text{52} \end{array}$ 
 $\begin{array}{c} \text{G20-G19} \\ \text{54} \end{array}$ 
 $\begin{array}{c} \text{G12} \\ \diagup \\ \text{N} \\ \diagdown \\ \text{G12} \end{array}$

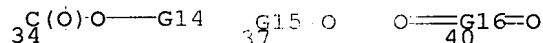
$$\begin{array}{c} \text{G17=O} \quad \text{O=O} \quad \text{G18 O} \\ \text{65} \quad \text{65} \\ \text{70} \text{C(O)-N} \text{---} \text{C(O)-NH-G21} \end{array}$$

Page 47

368866



G13 = OH / alkoxy<(1-3)> / CN / 34 / NO2 / F / Cl / Br /  
I / NH2 / alkylamino<(1-4)> / dialkylamino<(1-4)> / Ph (SO) /  
naphthyl (SO) / Hy<EC (1-3) Q (0-) N (0-) O (0-) S (0)  
OTHERQ, RC (1), RS (1) M5 (1) X7> / 37 / 40 /  
Hy<EC (1-3) Q (0-) N (0-) O (0-) S (0) OTHERQ (6-) C,  
AR (1-), BD (6-) N, RC (2), RS (0-) E5 (1-) E6 (0-) E7 (0)  
OTHER>



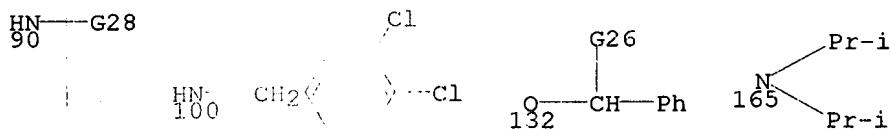
G14 = H / alkyl<(1-4)> (SO) / Ph (SO) / naphthyl (SO)  
G15 = Hy<EC (1-3) Q (0-) N (0-) O (0-) S (0) OTHERQ,  
RC (1), RS (1) M5 (1) X7> / Hy<EC (1-3) Q (0-) N (0-) O (0-)  
S (0) OTHERQ (6-) C, AR (1-), BD (6-) N, RC (2),  
RS (0-) E5 (1-) E6 (0-) E7 (0) OTHER>  
G16 = Hy<EC (1-3) Q (0-) N (0-) O (1-) S (0) OTHERQ,  
AN (1-) S, RC (1), RS (1) M5 (1) X7> /  
Hy<EC (1-3) Q (0-) N (0-) O (1-) S (0) OTHERQ (6-) C,  
AN (1-) S, AR (1-), BD (6-) N, RC (2),  
RS (0-) E5 (1-) E6 (0-) E7 (0) OTHER>  
G17 = Hy<EC (1-3) Q (0-) N (0-) O (0-) S (0) OTHERQ,  
RC (1), RS (1) M5 (1) X7> (SO) /  
Hy<EC (1-3) Q (0-) N (0-) O (0-) S (0) OTHERQ (6-) C,  
AR (1-), BD (6-) N, RC (2), RS (0-) E5 (1-) E6 (0-) E7 (0)  
OTHER> (SO)  
G18 = Hy<EC (1-3) Q (0-) N (0-) O (1-) S (0) OTHERQ,  
AN (1-) S, RC (1), RS (1) M5 (1) X7> (SO) /  
Hy<EC (1-3) Q (0-) N (0-) O (1-) S (0) OTHERQ (6-) C,  
AN (1-) S, AR (1-), BD (6-) N, RC (2),  
RS (0-) E5 (1-) E6 (0-) E7 (0) OTHER> (SO)  
G19 = alkyl<(1-3)> (SO) (1-) G13 / Ph (SO) /  
naphthyl (SO) / Hy<EC (1-3) Q (0-) N (0-) O (0-) S (0)  
OTHERQ, RC (1), RS (1) M5 (1) X7> (SO) / 57 / 60 /  
Hy<EC (1-3) Q (0-) N (0-) O (0-) S (0) OTHERQ (6-) C,  
AR (1-), BD (6-) N, RC (2), RS (0-) E5 (1-) E6 (0-) E7 (0)  
OTHER> (SO)



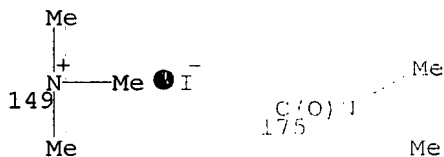
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G17=O      O= G18

```
G20      = S / S(0) / SO2
G21      = H / alkyls (1-5) / CH2Ph / cyclohexyl
G22      = O / S
G23      = 132 / 50 / OH / OEt / 100 / NHPh / NH2 / 165
```



G24 = Ph / NO2 / NH2 / NHCOMe / CN / CONH2 / NMe2 / 149 / OMe / 175



G25 = 2-pyridyl / Ph  
G26 = H / Ph  
G27 = COMe / CH(OH)Me / Bu-t  
G28 = 91 / 1-adamantyl / Bu-i / CH<sub>2</sub>CH<sub>2</sub>OH

p-C<sub>6</sub>H<sub>4</sub>G27

```
G29      = CN / NO2 / CONH2
G30      = CN / CONH2
G1 +G2   = NULL
G3 +G4   = NULL
DER:     or pharmaceutically acceptable salts or esters
MPL:     claims
NTE:     substitution is restricted
```

368866

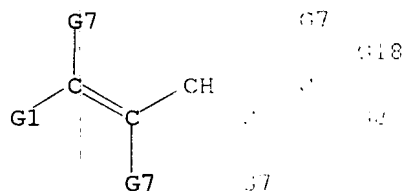
(ALL HITS ARE ITERATION INCOMPLETES)

ACCESSION NUMBER: 116:13416 MARPAT  
 TITLE: Pressure- and heat-sensitive recording materials with good sensitivity, storability and image stability  
 INVENTOR(S): Sano, Masajiro; Takashima, Masanobu; Satomura, Masato  
 PATENT ASSIGNER: Fuji Photo Film Co., Ltd., Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 11 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNTRY: 1  
 PATENT INFORMATION:

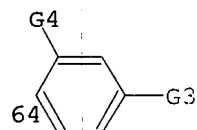
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 03142277	A2	19910618	JP 1989-282319	19891030

AB The title materials utilizes coloration by contact between electron-donating leuco dye Ar1R1CH:CR2:CH:CHR3CR4R5Ar2 (Ar1, Ar2 = amine residue-contg. aryl or heterocyclic group; R1-4 = H, monovalent group; R5 = aryl group, alkyl, alkoxy group; R1-4 may bond together forming 4- to 12-membered rings with or without contg. heteroatom) and electron-accepting compd.

MSTR 1B ITERATION INCOMPLETE



G1 = aryl (Rk (1 G2) / (EX 64)

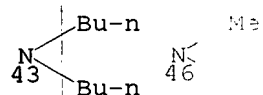


G2 = (1-) OR SO / R / (EX alkyl / alkoxy / aryloxy / X / OR / CH / 73 / alkylthio / arylsulfonyl / Ph)

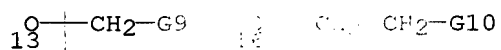
368866

G5-G6  
73

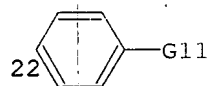
G3 = NMe2 / NEt2 / 43 / 46 / pyrrolidino



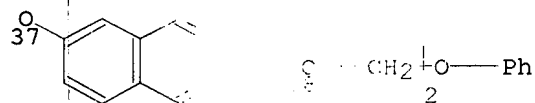
G4 = H / OPh / Me / Cl  
G5 = C(O) / SO2  
G6 = NH2 (SP) / OH (SR)  
G7 = H / R  
G8 = alkoxy (SP) / (EX 13 / 16)



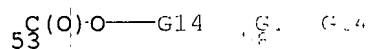
G9 = 22 / pyridyl



G10 = OPh / Ph / 3 / 38 / SPh



G11 = H / Cl / Br  
G12 = aryl / R / (EX 54 / 53)



368866

G13 = O / S / S O) / SO2 / C(O) / NH / 56

N—G15  
56

G14 = alkyl (G16) / aryl  
G15 = alkyl acyl  
G16 = aryl / R / (68 / 71)

C(O)O—G17  
68

G17 = alkyl (SO) / aryl  
G18 = Hy (SR) (L)  
MPL: claim

=>

---Logging off at 12:26:41---

=>

Executing the logoff script...

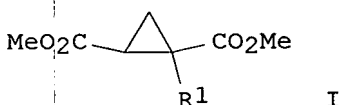
=> LOG Y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	204.78	331.53
DISCOUNT AMOUNT (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-4.24	-4.24

STN INTERNATIONAL LOGOFF AT 12:26:41 ON 20 JUL 2000

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LA English  
OS CASREACT 124:261655  
GI

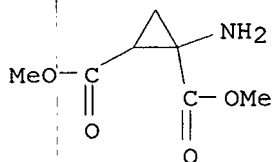


AB Aminolysis of bromocyclopropane diester I (R<sub>1</sub> = Br) in the presence of potassium hexamethyldisilazane (KHMDs) was investigated. Methoxycyclopropane diester I (R<sub>1</sub> = OMe) instead of the putative aminocyclopropane diester I (R<sub>1</sub> = NH<sub>2</sub>) was isolated from the reaction.

IT **175089-77-7P**  
RL: PNU (Preparation, unclassified); PREP (Preparation)  
(attempted synthesis of aminocyclopropanedicarboxylic acid via aminolysis of bromocyclopropanedicarboxylate)

RN 175089-77-7 CAPLUS

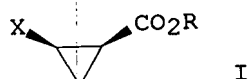
CN 1,2-Cyclopropanedicarboxylic acid, 1-amino-, dimethyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2000 ACS  
AN 1993:603875 CAPLUS  
DN 119:203875  
TI Preparation of cis-2-aminocyclopropanecarboxylic acid derivatives as intermediates for endothelin antagonist peptides  
IN Ishikawa, Kyobumi; Niiyama, Kenji; Ihara, Masaki; Yano, Mitsuo  
PA Banyu Pharma Co Ltd, Japan  
SO Jpn. Kokai Tokkyo Koho, 8 pp.  
CODEN: JKXXAF  
DT Patent  
LA Japanese  
FAN.CNT 1  
PATENT NO. KIND DATE APPLICATION NO. DATE

368866

PI	JP 05155827	A2	19930622	JP 1991-350316	19911209
OS	MARPAT 119:203875				
GI					



AB The title derivs. I (X = NX<sub>3</sub>X<sub>4</sub>; R = protective group; X<sub>3</sub>-4 = H, protective group) or their salts are prepd. from I (X = CO<sub>2</sub>H) by conversion to I (X = COX<sub>1</sub>; X<sub>1</sub> = NH<sub>2</sub>, N<sub>3</sub>), rearrangement into isocyanate derivs., hydrolysis or alcoholysis to I (X = NHX<sub>2</sub>; X<sub>2</sub> = H, alkoxycarbonyl) or their salts, and optional removal of the amino and/or the carboxy protective groups and/or protection of the amino group. Treating 2.88 g (-)-(1S,2R)-I (X = CO<sub>2</sub>Me, R = H) (prepn. given) with isobutylene and H<sub>2</sub>SO<sub>4</sub> in CH<sub>2</sub>Cl<sub>2</sub> at room temp. for 20 h gave 3.24 g diester, which was hydrolyzed by aq. K<sub>2</sub>CO<sub>3</sub> in MeOH to give 2.4 g (+)-(1S,2R)-I (X = CO<sub>2</sub>H, R = CMe<sub>3</sub>) (II). Stirring a suspension of 1.10 g II, NH<sub>4</sub>Cl, 1-hydroxy-1H-benzotriazole, Et<sub>3</sub>N, and 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide-HCl in DMF at room temp. for 5 h gave 0.91 g (+)-(1S,2R)-I (X = CONH<sub>2</sub>), reaction of 0.37 g of which with (CF<sub>3</sub>CO<sub>2</sub>)<sub>2</sub>Ph in MeCN in the presence of pyridine and subsequent reaction with Me<sub>3</sub>COH gave 0.25 g (1S,2R)-I (X = NHCO<sub>2</sub>CMe<sub>3</sub>, R = CMe<sub>3</sub>).

IT **150626-49-6P 150737-97-6P**  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of, as intermediate for endothelin-antagonizing peptides)

RN **150626-49-6 CAPLUS**  
 CN Cyclopropanecarboxylic acid, 2-amino-, 1,1-dimethylethyl ester, (1R-cis)-  
 (9CI) (CA INDEX NAME)

Absolute stereochemistry.

